Renormalized mean-field t-J model of high-T_c superconductivity: comparison with experiment

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Using an advanced version of the renormalized mean-field theory (RMFT) for the t-J model, we examine spin-singlet superconducting (SC) state of $d_{x^2-y^2}$-symmetry. Overall doping dependence of the SC gap magnitude is in good agreement with experimental results for $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) and $La_{2-x}Sr_xCuO_4$ (LSCO) compounds at the optimal doping and in the overdoped regime. We also calculate the dispersion relation for the Bogoliubov quasiparticles and compare our findings both with the angle resolved photoemission data for the cuprates, as well as with the variational Monte Carlo and other mean-field studies. Within the method proposed by Fukushima [cf. Phys. Rev. B **78**, 115105 (2008)], we analyze different forms of the t-J Hamiltonian, i.e. modifications caused by the form of exchange interaction, and by the presence of three-site terms. It is shown that although the former has a small influence, the latter suppresses strongly the superconductivity. We also analyze the temperature dependence of the gap magnitude and compare the results with those of the recently introduced finite-temperature renormalized mean-field theory (TRMFT) of Wang et al. [cf. Phys. Rev. B **82**, 125105 (2010)].

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I. INTRODUCTION

One of the most characteristic features of high temperature superconductivity (SC) is that upon hole doping, with the hole concentration $x \gtrsim 0.05$, a generic antiferromagnetic Mott insulating state of e.g. La_2CuO_4[1,2] transforms into SC state. The latter, in turn, after reaching a maximal transition temperature at $x \approx 0.15$, disappears at the upper critical concentration $x_c \gtrsim 0.25 - 0.35$, depending on the system.[3,4] The last property is particularly surprising, since in the overdoped regime $x \gtrsim 0.15$ the system evolves gradually from a non-Fermi liquid into a quantum liquid that can be regarded as an unconventional Fermi liquid.[5] The appearance of x_c may speak in favor of real-space type of pairing, as the increased hole doping reduces the pairing correlations in real space. To describe the above features the t-J model is often invoked,[6–8] and the kinetic exchange interaction is claimed to induce both antiferromagnetism and the superconductivity.[9]

The basic question is whether within the renormalized mean-field theory (RMFT)[10,11] we can reproduce at least some of the above properties in a semiquantitative manner,[11–13] as advocated strongly.[12,13] On the other hand, variational Monte Carlo (VMC) methods, within which one treats exactly the double occupancy exclusion, is known[14–19] to provide a semiquantitative description of the SC correlated state. Hence it is often regarded as being superior to any mean-field (MF) treatment. However, a proper MF approach would have important advantages over VMC. First, its results are not limited to small clusters. Second, it can offer an analytic insight into the physical contents of the model. Third, it allows for a detailed comparison with experiment or, strictly speaking, its critical assessment, as detailed below.

Numerous attempts to improve RMFT have been made,[20–23] in order to take into account also intersite correlations. Here we show that within the MF renormalization scheme proposed recently by Fukushima,[22] supplemented with the maximum-entropy based[24] self-consistent variational approach,[25–27] we can produce, among others, the results that are competitive to those of VMC. Specifically, the upper critical concentration x_c, as well as the principal features of the excitation spectrum, are shown to agree quite well with experiment in the overdoped regime. Finally, motivated by a recent paper,[28] we comment on the extension of the present treatment to finite temperatures. We study a behavior of the renormalized gap magnitude as a function of the temperature, which is shown to be in quite good agreement with the classic result of the BCS theory.

II. MODEL AND METHOD

We start from t-J model[6–9] is expressed by the following Hamiltonian

$$\hat{H}_{tJ} = \hat{P}\Big(\hat{H}_t + \sum_{\langle ij\rangle} J_{ij}\ \big(\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{c_1}{4}\hat{\nu}_i\hat{\nu}_j\big) + c_2\hat{H}_3\Big)\hat{P}. \quad (1)$$

The first term, $\hat{H}_t = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}$ is the kinetic energy part, the second expresses the kinetic exchange, and the third the three-site terms. $\sum_{\langle ij\rangle}$ means the summation pair of sites $\langle i, j\rangle$ (bonds). The Gutzwiller projector $\hat{P} = \prod_i (1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$ eliminates double occupancies in real space. Also, explicitly

$$\hat{H}_3 = \sum_{ijk\sigma} \frac{t_{ij}t_{jk}}{U}\left(b^\dagger_{i\sigma}\hat{S}^{\bar{\sigma}}_j b_{k\bar{\sigma}} - b^\dagger_{i\sigma}\hat{\nu}_{j\bar{\sigma}} b_{k\sigma}\right), \quad (2)$$

with the projected fermion operators defined as: $b_{i\sigma} \equiv (1-\hat{n}_{i\bar{\sigma}})c_{i\sigma}$, $\hat{\nu}_{i\sigma} \equiv (1-\hat{n}_{i\bar{\sigma}})\hat{n}_{i\sigma}$, $\hat{\nu}_i \equiv \sum_\sigma \hat{\nu}_{i\sigma}$, and $\hat{S}_i^\sigma \equiv b_{i\sigma}^\dagger b_{i\bar{\sigma}}$. Here the standard fermion creation (annihilation) operators are $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) and $\hat{n}_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$. Hamiltonian (1) in its complete form, i.e. with $c_1 = c_2 = 1$ is derived by applying canonical transformation to the Hubbard Hamiltonian, $\hat{H}_{tU}$, in the strong coupling ($|t| << U$) limit,[6,7] $\hat{H}_{tJ} = \exp(-iS)\hat{H}_{tU}\exp(iS)$. Then, kinetic exchange integral $J_{ij} = 4|t_{ij}|^2/U$. On the other hand, the $c_1 = c_2 = 0$ case has been used as a simplified effective model describing low-energy sector of a multi-band Hubbard model.[8,9] Both the latter form, or that with $c_1 = 1$, $c_2 = 0$, are often used in studies of high- T_c superconductivity. Our aim here is, among others, to compare the complete version of the t-J model with the simpler forms.

It has been argued,[12] that a correct variational state describing the ground state of the t-J Hamiltonian is of the form $|\Psi\rangle = \hat{P}|\Psi_0\rangle$, where $|\Psi_0\rangle$ is an uncorrelated state, here taken as the Bardeen-Cooper-Schrieffer (BCS)-type state. When the Hubbard model is the starting point of analysis, the re-transformed back state with perturbatively reintroduced double occupancies is used instead, i.e $|\Psi\rangle \to |\tilde{\Psi}\rangle = \exp(iS)|\Psi\rangle$.[13,14] Also, the detailed form of $|\Psi_0\rangle$ may be postulated without specifying the underlying microscopic Hamiltonian.[12] However, within RMFT, $|\Psi_0\rangle$ may also be selected as an eigenstate of the effective single-particle Hamiltonian, obtained from the mean-field treatment of (1).[10,11,20,21] This point of view is also taken up here.

Construction of RMFT requires a prescription (here called the renormalization scheme, RS) for calculating expectation value of an arbitrary operator $\hat{\mathcal{O}}$ in the correlated state $|\Psi\rangle$. Explicitly,

$$\langle\hat{\mathcal{O}}\rangle_C \equiv \frac{\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi_0|\hat{P}_C\hat{\mathcal{O}}\hat{P}_C|\Psi_0\rangle}{\langle\Psi_0|\hat{P}_C^2|\Psi_0\rangle} \equiv \frac{\langle\hat{P}_C\hat{\mathcal{O}}\hat{P}_C\rangle}{\langle\hat{P}_C^2\rangle}. \tag{3}$$

In the above, the projector $\hat{P}$ has been replaced by more general correlator $\hat{P}_C$, which differs from $\hat{P}$ by the presence of fugacity factors, ensuring that the projected and preprojected average particle numbers are equal, i.e. $\langle\hat{n}_{i\sigma}\rangle_C = \langle\hat{n}_{i\sigma}\rangle$.[22]

We adopt the RS of Ref. 22 and supplement it with the variational formalism proposed recently by us.[25,26] Combination of these two factors yields the results that differ considerably as compared to those of the standard RMFT.[10,11] To carry out the self-consistent variational approach, we start from the following effective MF grand Hamiltonian

$$\begin{aligned}\hat{K}_\lambda &= -\sum_{\langle ij\rangle\sigma}\Big(\tilde{\eta}_{ij\sigma}\big(c_{i\sigma}^\dagger c_{j\sigma} - \chi_{ij\sigma}\big) + \text{H.c.}\Big) \\ &- \sum_{\langle ij\rangle}\Big(\tilde{\gamma}_{ij}\big(\hat{\Delta}_{ij} - \Delta_{ij}\big) + \text{H.c.}\Big) - \mu\sum_{i\sigma}\hat{n}_{i\sigma} \\ &- \sum_{i\sigma}\big(\tilde{\lambda}_{i\sigma}^n\big(\hat{n}_{i\sigma} - n_{i\sigma}\big)\Big) + W(\chi_{ij\sigma}, \Delta_{ij}, n_{i\sigma}),\end{aligned} \tag{4}$$

with $\hat{K}_\lambda \equiv \hat{H}_\lambda - \mu\hat{N}$, $W \equiv \langle\hat{H}_{\text{tJ}}\rangle_C$, $n_{i\sigma} \equiv \langle\hat{n}_{i\sigma}\rangle$, $\chi_{ij} \equiv \langle c_{i\sigma}^\dagger c_{j\sigma}\rangle$, $\hat{\Delta}_{ij} \equiv (c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow})/2$, and $\Delta_{ij} \equiv \langle\hat{\Delta}_{ij}\rangle$. The averages $\langle\ldots\rangle$ are defined by (3) for zero temperature, or in general, with the help of density operator $\hat{\rho}_\lambda$, (see below). $\tilde{\eta}_{ij\sigma}$, $\tilde{\gamma}_{ij}$, and $\tilde{\lambda}_{i\sigma}^n$ (not to be confused with the fugacity factors of Ref. 22) are the Lagrange multipliers, ensuring the self-consistency of this variational approach, as this is not guaranteed within the standard Gutzwiller approximation.[27] The form (4), apparently different from the usual formulation of RMFT, is fully equivalent to it (a similar approach is discussed in Ref. 23).

We solve this model on a square lattice and in the spatially homogeneous situation, with no coexisting magnetic order. The model parameters are $t_1 \equiv t, t_3 \equiv t'$ and $t_5 \equiv t''$, where $s = 1, 3, 5$ corresponds to sites located at the distances $d(i,j)$ of $1, \sqrt{2}$, and 2 lattice constants, respectively. Consequently, the following Lagrange multipliers and the corresponding mean fields are assumed as nonzero: $\chi_{ij} = \xi_s$ and $\eta_{ij} = \eta_s$; $\Delta_{ij} = \Delta_{x(y)}$, with $\Delta_x = \Delta = -\Delta_y$ and $\tilde{\gamma}_{ij} = \gamma_{x(y)} = \pm\gamma$, both for $d(i,j) = 1$; $n_{i\sigma} = n_{i\bar{\sigma}} = n/2$ and $\tilde{\lambda}_{i\sigma}^n = \lambda$. Also, in (1) we retain all the terms of the orders of t^2/U and tt'/U, and neglect a smaller term of the order $(t')^2/U$. Then, $\langle\hat{H}_{tJ}\rangle_C$ is obtained using the formalism of Ref. 22. Explicitly,

$$W = \langle\hat{H}_t\rangle_C + \langle\hat{H}_J\rangle_C + \langle\hat{H}_3\rangle_C \equiv W_t + W_J + W_3, \tag{5}$$

where $W_J = \tilde{W}_J - \Lambda J c_1 n^2/2$, and Λ is the number of lattice sites. In effect, we have that

$$\begin{aligned}\frac{W_t}{\Lambda} &= \frac{16(1-n)}{2-n}\Big\{t_1\xi_1\left(1 - \frac{4(\Delta^2+\xi_1^2)}{(2-n)^2}\right) \\ &+ \sum_{s=3,5} t_s\xi_s\left(1 - \frac{4\xi_s^2}{(2-n)^2}\right)\Big\},\end{aligned} \tag{6}$$

$$\frac{\tilde{W}_J}{\Lambda} = -4J\left(\frac{3\left(\Delta^2+\xi_1^2\right) + c_1(1-n)^2\left(\Delta^2-\xi_1^2\right)}{(2-n)^2}\right). \tag{7}$$

The formula for W_3, containing three-site terms, is too lengthy to be reproduced here.

The next step is the diagonalization of $\hat{H}_\lambda$ (4) via Bogoliubov-Valatin transformation, which leads to

$$\hat{K}_\lambda = \sum_{\mathbf{k}} E_{\mathbf{k}}(\hat{\gamma}_{\mathbf{k}0}^\dagger\hat{\gamma}_{\mathbf{k}0} + \hat{\gamma}_{\mathbf{k}1}^\dagger\hat{\gamma}_{\mathbf{k}1}) + \sum_{\mathbf{k}}(\xi_{\mathbf{k}} - E_{\mathbf{k}}) + C, \tag{8}$$

with $C = W + \Lambda(8\sum_s \xi_s\eta_s + 4\Delta\gamma + \lambda n)$. Also, the quasiparticle energy $E_{\mathbf{k}}$, the renormalized gap $D_{\mathbf{k}}$, and the renormalized band energy $\xi_{\mathbf{k}}$ are respectively given by

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + D_{\mathbf{k}}^2}, \quad D_{\mathbf{k}} = -\frac{\gamma}{2}\Gamma_-(\mathbf{k}), \tag{9}$$

$$\xi_{\mathbf{k}} = -\left(\eta_1\Gamma_+(\mathbf{k}) + \eta_3\Theta(\mathbf{k}) + \eta_5\Gamma_5(\mathbf{k}) + \tilde{\mu}\right), \tag{10}$$

$\Gamma_{\pm}(\mathbf{k}) = 2(\cos(k_x) \pm \cos(k_y))$, $\Theta(\mathbf{k}) = 4\cos(k_x)\cos(k_y)$, $\Gamma_5(\mathbf{k}) = 2(\cos(2k_x) \pm \cos(2k_y))$, and $\tilde{\mu} \equiv \mu + \lambda$. Then, the corresponding grand-canonical density operator reads

$$\hat{\rho}_\lambda = \mathcal{Z}_\lambda^{-1} \exp(-\beta \hat{K}_\lambda), \tag{11}$$

with $\mathcal{Z}_\lambda = \mathrm{Tr}[\exp(-\beta \hat{K}_\lambda)]$, $\beta = 1/k_B T$, and the generalized Landau functional, $\mathcal{F} \equiv -\beta^{-1} \ln \mathcal{Z}_\lambda$ reads

$$\mathcal{F} \;=\; C + \sum_{\mathbf{k}} \left((\xi_{\mathbf{k}} - E_{\mathbf{k}}) - \frac{2}{\beta} \ln\left(1 + e^{-\beta E_{\mathbf{k}}}\right) \right). \tag{12}$$

Because of extra constraints in (4), the necessary conditions for $\mathcal{F}$ to have a minimum are

$$\partial_w \mathcal{F} = 0, \quad \partial_z \mathcal{F} = 0, \tag{13}$$

for the mean-fields $w \in \{\xi_s, \Delta, n\}$, $n \equiv 1 - x$, and the Lagrange multipliers $z \in \{\eta_s, \gamma, \lambda\}$. In contrast to our previous formulation,[25] the equations $\partial_w \mathcal{F} = 0$ are solved analytically, but the solution of those remaining ($\partial_z \mathcal{F} = 0$) must be determined numerically. Optimal values of the mean-fields and the Lagrange multipliers, given by a solution of (13) characterized with the lowest value of $\mathcal{F}$ and denoted respectively $(\xi_1^{(0)}, \xi_3^{(0)}, \xi_5^{(0)}, \Delta^{(0)}, n) \equiv \vec{A}_0(T, V, \mu)$, $(\eta_1^{(0)}, \eta_3^{(0)}, \eta_5^{(0)}, \gamma^{(0)}, \lambda^{(0)}) \equiv \vec{\lambda}_0(T, V, \mu)$, may be used next to construct standard grand thermodynamic potential Ω and the free energy $F = \Omega + \mu N$. Explicitly,

$$\Omega(T, V, \mu) = \mathcal{F}(T, V, \mu; \vec{A}_0(T, V, \mu), \vec{\lambda}_0(T, V, \mu)). \tag{14}$$

The present formalism, based on the maximum-entropy principle[24] is formally valid for arbitrary $T > 0$. Consequently, we have replaced pure state $|\psi_0\rangle$ by mixed state represented by $\hat{\rho}_\lambda$. However, the solutions obtained for non-zero, but sufficiently low T, are for all practical purposes identical to those for $T = 0$. This situation is studied in the next Section. The separate question is that of the validity of RMFT approach at $T > 0$ from the point of view of physical consistency. This is analyzed in more detail in Section IV.

III. RESULTS FOR $T \approx 0$

An analytical expression for $W = \langle \hat{H}_{tJ} \rangle_C$ allows us to make qualitative predictions before the numerical analysis is carried out. First, from (6) we expect a strong tendency to the superconductivity suppression for higher doping, as SC order leads to the band energy decrease $\sim \Delta^2$. On the other hand, in that regime the renormalized band energy becomes predominant over the exchange part. In effect, the normal state is favored over SC for $x > x_c$ with x_c smaller than obtained within previous MF treatments.[10–13,16] Second, from (7) we infer, that the influence of the $\hat{\nu}_i \hat{\nu}_j/4$ term on W_J is small except for the largest doping; this is due to the presence of the $(1-n)^2$ prefactor (the other term $\sim n^2$ merely shifts the chemical potential). On the other hand, W_3 is multiplied only by $(1 - n) = x$ prefactor. Consequently, for higher x this term becomes rather important, due to the number of distinct three-site terms present for a given initial site and spin direction (eight for $d(i,j) = \sqrt{2}$, and four for $d(i,j) = 2$). Also, this part of W is expected to suppress SC order, as the term $\sim \Delta^2$ in W_3 contains a factor, which is positive for reasonable values of other mean fields and model parameters.

We solve numerically the part $\partial_z \mathcal{F} = 0$ of Eqs. (13) for the mean fields using periodic boundary conditions on the lattice of $\Lambda = 512^2$ sites, to minimize finite size effects and for low temperature $k_B T = 2 \cdot 10^{-3} J$. The solution amounts to solving simultaneously the system of five nonlinear equations using GNU Scientific Library (GSL). In the most cases we take the parameters $|t|/J = 3$ (corresponding to $U/|t| = 12$ for the Hubbard model), $t'/t = 0$ or (-0.25), and $t'' = 0$. Additionally, we take also $|t| = 0.3$ eV or $|t| = 0.4$ eV, which correspond roughly to the lower and the upper limits of the realistic values of this parameter, depending on the compound. Values of $|t|$ close to 0.4 eV have been determined from the band-structure calculations,[9,29] whereas $|t| = 0.3$ eV is used in Refs. 13,14. To highlight the influence of various forms of (1), the results for different values of c_1 and c_2 are analyzed. The numbers 1, 2, 3 (4, 5, 6) in Figs. 1-4 and Table I correspond to the three situations: $c_1 = c_2 = 0$ (i.e. with the $\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$ part of the kinetic exchange only, cf. (1)), $c_1 = 1$ and $c_2 = 0$ (with full form of the kinetic exchange), and $c_1 = c_2 = 1$ (complete form of the t-J Hamiltonian with the three-site terms included), each case taken for $t'/t = 0$ ($t'/t = -0.25$), respectively.

In Table I we provide the equilibrium values of the mean-fields and of the Lagrange multipliers for cases 1-6 and for $x = 0.175$, a representative hole concentration in the overdoped regime.

Table I. Optimal values of mean-field parameters for $T \approx 0$ and $x = 0.175$.

φ	1	2	3	4	5	6
ξ_1	0.1970	0.1969	0.1990	0.1924	0.1922	0.1944
ξ_3	0.0468	0.0465	0.0505	0.0241	0.0239	0.0225
ξ_5	-0.0080	-0.0076	-0.0144	0.0337	0.0340	0.0383
Δ_x	0.0687	0.0708	0.0202	0.0903	0.0919	0.0534
η_1	1.0080	1.0030	1.2355	1.0031	0.9982	1.1845
η_3	0.0000	0.0000	0.0803	-0.2223	-0.2223	-0.2118
η_5	0.0000	0.0000	0.0408	0.0000	0.0000	0.0404
$\tilde{\gamma}_x$	0.1584	0.1665	0.0320	0.2126	0.2205	0.0834
$\tilde{\mu}$	-0.4069	-0.4080	-0.2935	-0.8633	-0.8614	-0.9406

In Fig. 1 we plot the dispersion relation for the Bogoliubov quasiparticles, calculated for the parameters displayed in Table I. The influence of $\hat{H}_3$ on $E_{\mathbf{k}}$ is of comparable magnitude to that of having nonzero t'.

Next, we discuss the doping-dependence of the renormalized SC order parameter $\langle \hat{\Delta}_{ij} \rangle_C \equiv \Delta_C$ (cf. Eqn. (18) of Ref. 22). The numerical results confirm the above

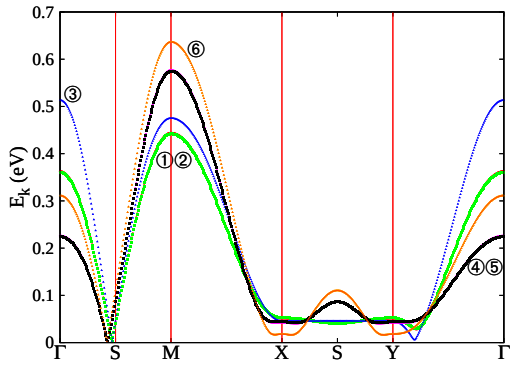

FIG. 1: (Color online) Dispersion relations along the main symmetry lines in the two-dimensional Brillouin zone for $n = 0.825$. The various curves are explained in main text. Note, the curves 1 and 2, as well as 4 and 5 are practically indistinguishable (the influence of the term $\sim c_1$ in (1) is neglible).

made qualitative predictions. In Fig. 2 we plot Δ_C for the cases 1-6 specified above, as well as for $t'/t = -0.27$ (value being reasonable for BSCCO compounds,[30]) and $J/|t| = 0.3$ (curve 7). Note, that the upper criti-

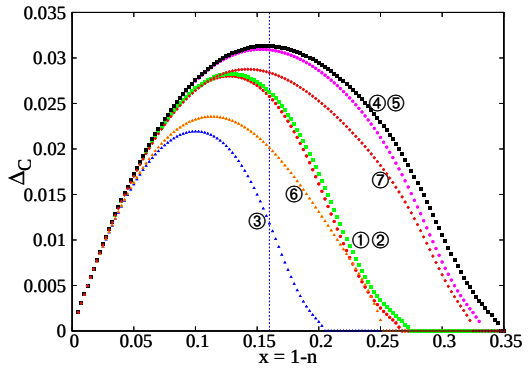

FIG. 2: (Color online) Doping dependence of the renormalized superconducting order parameter $\langle\hat{\Delta}\rangle_C \equiv \Delta_C$. The curves 1-6 correspond to those in Fig. 1. The curve 7 is for $c_1 = 1$, $c_2 = 0$, $t'/t = -0.27$, $t'' = 0$, and for $J/|t| = 0.3$. For definitions of cases 1-7 see the main text. Cases 3 and 6 correspond to the complete t-J Hamiltonian (1) with $c_1 = c_2$.

cal concentration x_c for the cases 4 and 5 is close to the VMC result,[14] obtained within the Hubbard model and using $|\tilde{\psi}\rangle$ for the corresponding model parameters. Also, nonzero value of t' enhances superconductivity, in agreement with previous VMC results[16] and other calculations.[30] Let us emphasize again, that the presence of the $\hat{H}_3$ term acts in the opposite direction. The vertical line roughly marks the boundary between under- and over-doped regimes. Importantly, for $|t|/J = 3$, $t'' = 0$ and different t'/t values, $0 \le t'/t \le 0.25$, x_c lies in the interval $0.2 \lesssim x_c \lesssim 0.35$, depending on the form of $\hat{H}_{\rm tJ}$, as illustrated in Fig. 2. As said above, the small difference between the curves 4 and 5 (as well as between 1 and 2) shows an insignificane of the term $\sim c_1$ (cf. also Table I). The results for x_c are in a good overall agreement with the experimental data for the cuprates.[4,9] To provide an additional support for our results, we list in Table II the values of x_c as a function of J, for either $t'/t = -0.1$ (considered to be relevant to the LSCO compound[9]), or $t'/t = -0.27$.

A remark is in place here. The family of curves in Fig. 2 and of x_c values in Table II has the following meaning. Each x_c value singles out either the choice of a model or a particular set of parameters. This detailed analysis is to illustrate that there is a clear upper critical concentration in the proper range, irrespectively of the model details or particular set of parameter values.

Table II. Upper critical concentration x_c vs. J for $t' = -0.27t$ or $t' = -0.1t$. The symbol A (B) labels the case $c_2 = 0$ and $c_1 = 0$ ($c_1 = 1$), respectively, whereas C means that $c_1 = c_2 = 1$ is taken in the computation.

$J/\|t\|$	0.2	0.3	0.333	0.375	0.4
$t'/t = -0.1$ A	0.18	0.26	0.29	0.32	0.33
$t'/t = -0.27$ A	0.2	0.31	0.34	0.38	0.4
$t'/t = -0.1$ B	0.18	0.27	0.3	0.33	0.35
$t'/t = -0.27$ B	0.2	0.33	0.36	0.4	0.42
$t'/t = -0.1$ C	0.15	0.21	0.22	0.24	0.25
$t'/t = -0.27$ C	0.15	0.23	0.26	0.28	0.29

In Fig. 3 we plot x-dependence of the SC gap $D_{\mathbf{k}}$ for $\mathbf{k} = (\pi, 0)$ (c.f. Eqn. (9)) and compare our results with the experimental data.[31] For the selections of t'/t and $J/|t|$ as in Fig. 1, no fully satisfactory agreement with experiment is achieved in the entire range of x. However, the agreement with experiment is quite good for the parameters corresponding to the curves 1, 2, 4 and 5 in the overdoped regime, both for $|t| = 0.3$ eV and $|t| = 0.4$ eV. The best overall fit is achieved for the set of parameters represented by curve 7. Note, that in all the cases 1-7 the quasiparticle energies obtained here are decisively lower than those in the standard RMFT formulation.[13] These differences are caused by both the particular selection of the renormalization scheme, as well as by the variational method we use. As a consequence, we obtain also lower values of the Fermi velocity, $v_F \equiv |\nabla_k \xi_{\mathbf{k}}|_{|\mathbf{k}|=k_F}$, calculated for the nodal $((0,0) \to (\pi,\pi))$ direction. The lattice constant has been taken as $a_0 = 4$Å.[13]

The x-dependence of v_F is detailed in Fig. 4 for the same set of parameters as in Figs. 2 and 3, for both $|t| = 0.3$ eV and $|t| = 0.4$ eV, and compared with the data discussed before.[13] The theoretical values are still too low. Also, the x-dependence of both $D_{\mathbf{k}=(\pi,0)}$ and v_F, obtained within the MF approaches, is stronger than observed in experiment. This feature is shared with the other mean-field approaches.[13,14] However, the experimental values for BSCCO ~ 1.5 eV Å have also been reported,[32] and are quite close to our results. Note that the disagreement is largest in the underdoped regime (to

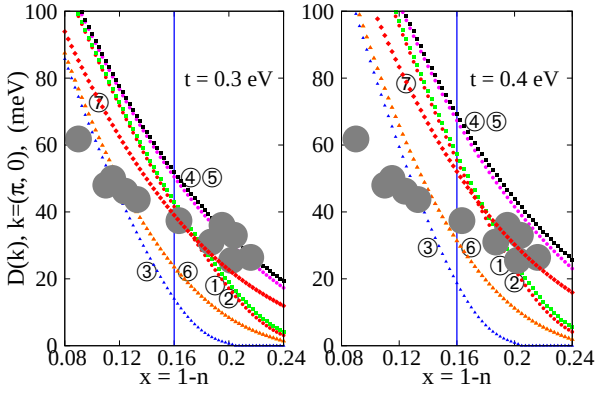

FIG. 3: (Color online) Doping dependences of the SC gap $D_{\mathbf{k}}$ at $\mathbf{k} = (\pi, 0)$ for cases 1-6 and for $t'/t = -0.27$, and $J/|t| = 0.3$ (filled diamonds). Large filled circles - experimental data.[31] Note, that in contradistinction to Ref.[13] no *ad hoc* introduced scaling factor $\alpha = 1/2$ is necessary to obtain a reasonable agreement in the overdoped regime, i.e. to the right of the vertical line.

the left of the vertical line).

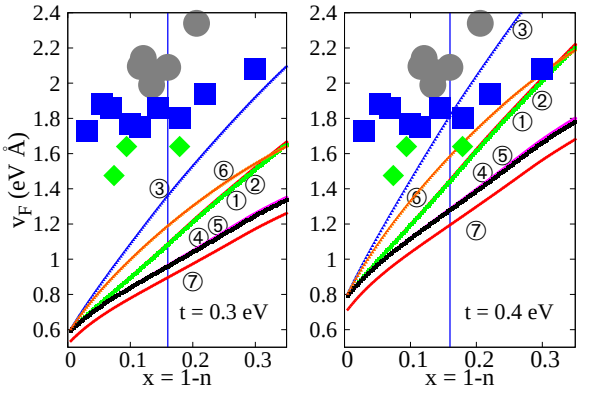

FIG. 4: (Color online) Doping dependence of Fermi velocity in the nodal ($(0,0) \to (\pi,\pi)$) direction. Experimental data (cf.[13] and References therein) are marked by diamonds (YBCO), squares (LSCO) and solid circles (BSCCO).

IV. RESULTS FOR $T > 0$.

So far, we have analyzed only low temperature $\beta J = k_B T/J = 500$, practically equivalent to the true $T = 0$ situation. Obviously, it would be interesting to extend the analysis for higher temperatures, and in particular, to determine the critical temperature T_c as a function of doping. Standard RMFT approach, as based on the Gutzwiller approximation (GA), is devised to study ground-state properties and as such, is not applicable directly for $T > 0$. It may seem, that having a finite-temperature formalism at our disposal, we may examine arbitrary temperature by simply changing value of β in $\mathcal{F}(\beta)$ Eq. (12). Unfortunately, this may lead to the situation similar to that encountered in the slave-boson mean-field theories, which application at finite temperatures is invalidated by incorrect evaluation of the entropy part of the free energy.[33]

Recently, an attempt to extend RMFT to $T > 0$ have been made.[28] Within this approach, termed *finite temperature RMFT* (TRMFT), the term

$$\Delta S = -\sum_i \left(e_i \ln \frac{e_i}{e_{i0}} + q_i \ln \frac{q_i}{q_{i0}} + d_i \ln \frac{d_i}{d_{i0}} \right). \quad (15)$$

is added to the single-particle entropy $S_0 = -\mathrm{Tr}\hat{\rho}_0 \ln \hat{\rho}_0$ of the mean-field model (here, $\hat{\rho}_0 = \hat{\rho}_\lambda$). In Eq. (15), we have $e_i = \langle \hat{E}_i \rangle_C$, $e_{i0} = \langle \hat{E}_i \rangle$, $q_i = \langle \hat{Q}_i \rangle_C$, $q_{i0} = \langle \hat{Q}_i \rangle$, $d_i = \langle \hat{D}_i \rangle_C$, and $d_{i0} = \langle \hat{D}_i \rangle$ with $\hat{E}_i = (1-\hat{n}_{i\uparrow})(1-\hat{n}_{i\downarrow})$, $\hat{Q}_i = \hat{n}_{i\uparrow}(1-\hat{n}_{i\downarrow}) + \hat{n}_{i\downarrow}(1-\hat{n}_{i\uparrow})$ and $\hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$. Note, that $\Delta S < 0$. Derivation of (15), and its possible generalizations will be discussed elsewhere.[34] Here we simply adapt Eq. (15), which may be treated as a reasonable *Ansatz*, similar in spirit to the finite-temperature extensions of the Gutzwiller approximation proposed earlier.[35–37]

Within the present formalism, ΔS can be included by replacing $W(\xi_s, \Delta, n)$ (5) by $W - T\Delta S$. However, for the t-J model, $d_i = 0$, and consequently, for non-magnetic, homogeneous solutions studied here, $\Delta S \equiv \Delta S_{tJ}$ depends only on the total particle number n, i.e.

$$\frac{\Delta S_{tJ}}{\Lambda} = (2-n)\ln\left(1-\frac{n}{2}\right) - (1-n)\ln(1-n). \quad (16)$$

Therefore, the presence of ΔS_{tJ} results only in different values of μ, λ, and thermodynamic potentials Ω and F (14). Still, $\tilde{\mu} = \mu + \lambda$, all the mean fields, and the remaining Lagrange multipliers, as well as the free energy difference between the superconducting and the normal solutions, remain unchanged. Hence, ΔS in the form (15) does not lead to any nontrivial modifications of our original formulation.

Nonetheless, it still seems to be interesting to apply the above formalism to examine nonzero temperature situation. This would reveal limitations of the present form of RMFT and should help in formulating more satisfactory finite-temperature mean-field treatment of the t-J model. First, in Fig. 5 we plot temperature dependence of (renormalized) gap magnitude $\Delta_C(T)$ as a function of T for selected hole concentrations. For the values of model parameters used here, we have $J = 100\mathrm{meV} \approx 1160\mathrm{K}$ ($J = 133\mathrm{meV} \approx 1550\mathrm{K}$) for $t = 300\mathrm{meV}$ ($t = 400\mathrm{meV}$), respectively. Therefore, the critical temperature is overestimated by a factor 3-5 (e.g. $T_c = 340 - 450\mathrm{K}$ at the optimal doping and $T_c \approx 25 - 35\mathrm{K}$ at $x = 0.3$. This is a common feature of all mean-field type approaches, clearly caused by neglecting the fluctuations. This also

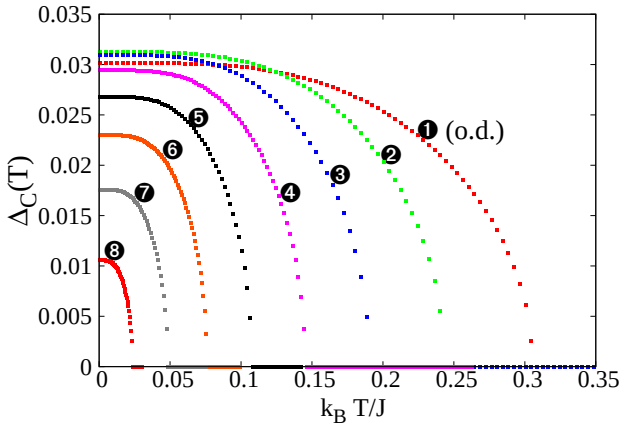

FIG. 5: (Color online) Temperature dependence of renormalized superconducting order parameter $\langle\hat{\Delta}\rangle_C(T) \equiv \Delta_C(T)$. The numbers 1-8 correspond to values of doping equal 0.125 (optimal doping, o.d.), 0.15, 0.175, 0.2, 0.225, 0.25, 0.275 and 0.3, all for $c_1 = 1$, $c_2 = 0$, $t'/t = -0.25$.

shows the insufficiency of the expression ΔS (15) in the present t-J model case.

Nonetheless, one interesting property of the present approach should be noted. Namely, an uncorrelated wave function $|\Psi_0\rangle$, or a related density operator $\hat{\rho}_\lambda$ (11) has an essentially the same form as that coming from the Bardeen-Cooper-Schrieffer (BCS) theory. Therefore, it seems natural to compare our values of reduced renormalized gap magnitude $\Delta_C(T)/\Delta_C(0)$ with the standard BCS result[38] given by $\Delta(T)/\Delta(0) = \tanh(\Delta(T)/t\Delta(0))$, where $t = T/T_C$. The results are shown in Fig. 6. Interestingly, the agreement with the BCS results is quite

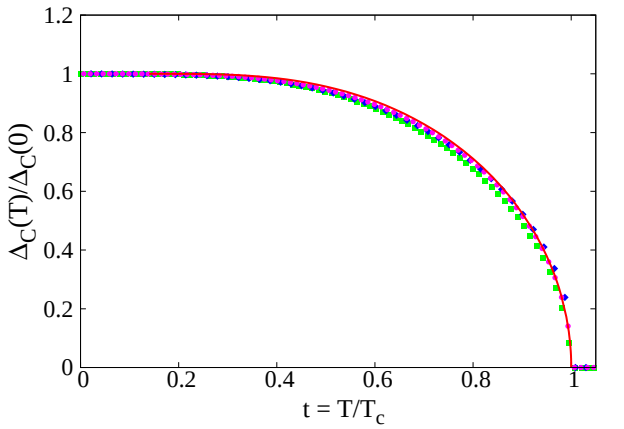

FIG. 6: (Color online) Reduced temperature dependence of renormalized superconducting order parameter $\langle\hat{\Delta}\rangle_C \equiv \Delta_C(T)$ for various doping levels. Squares: $x = 0.125$, solid circles: $x = 0.25$, diamonds: $x = 0.3$ are all for $c_1 = 1$, $c_2 = 0$, $t'/t = -0.25$. Solid line: BCS result.

good, despite the renormalization of Δ and its nontrivial d-wave symmetry. Uncorrelated (bare) gap ratio $\Delta(T)/\Delta(0)$ exhibits very similar scaling with T/T_c.

V. SUMMARY AND OUTLOOK

In this paper, we aimed to describe the doping dependences of selected, experimentally measured quantities, we have decided to systematize the results coming from different versions of t-J model, that are discussed in the literature. From that analysis it follows that while the presence of the term $\sim c_1$ does not influence remarkably the results except for the largest doping x, the inclusion of the three-site terms ($c_1 = c_2 = 1$) reduces substantially the range in which superconductivity is present.

We have implemented the mean-field renormalization scheme[22] to t-J model, in which both the kinetic-exchange and the three-site terms can be taken into account. Such RMFT approach, which is based on an effective single-particle picture, is expected to be valid first of all in the overdoped regime, where an unconventional form of the Fermi liquid is obtained. The variational approach based on the maximum entropy principle[24] has been used to determine mean-field parameters appearing in the model. The theoretical results yield a correct value for the upper critical concentration for the high-T_c d-wave superconductivity disappearance.

Our method provides also lower single-particle energies compared to the previous MF results.[13] Consequently, a good estimate of the experimentally determined gap $D_{\mathbf{k}=(\pi,0)}$ is detected experimentally in the overdoped regime for typical values of the model parameters. However, the values of the Fermi velocity in the nodal direction are still slightly too low. We also have examined the temperature dependence of the superconducting gap magnitude and have determined the critical temperature $T_c(x)$ evolution as a function of hole concentration. As may be expected, mean-field results overestimate T_c by a factor 3-5. The present results can be generalized by taking into account more complex lattice or band structure, the broken C_{4v} symmetry (Pomeranchuk instability[25]), and antiferromagnetism. Furthermore, study of the Fermi-surface-topology evolution with the doping is achievable. Finally, a more advanced scheme of calculating the entropy of the correlated state is desired to provide more satisfactory description of the nonzero-temperature situation. We should be able to see progress along these lines soon.

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